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AN A-STABLE MODIFICATION OF ADAMS-BASHFORTH's METHOD FOR THE NUMERICAL INTEGRATION OF ORDINARY STIFF DIFFERENTIAL EQUATIONS

by

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1. Introduction. Let us consider the differtial equation

(1.1) $y'(x) = f(x,y(x))$, $y(a) = \eta$

over the interval $[a,b]$, where $f \in C([a,b] \times \mathbb{R})$ and Lipschitz continous in the second variable. Then (1.1) has exactly one solution $y \in C^1([a,b])$.

Initial value problems for non-linear differential equations with large Lipschitz constants are encountered in many applications. But it often happens that the solution is smooth outside a transient phase, inside which there is a rapid variation. It is convenient to refer to the general class of problems exhibiting this behavior as stiff .

In integrating stiff equations with a k-step multistep method, we have for obtaining the desired accuracy in the transient phase, to choose a very small step h . When this phase is over, we would then like to proceed with a much greater step h , since the solution in this part of the integration interval is smooth. But, in general for a k-step method we have to impose a strict condition on h , a restriction which might turn out to be prohibitive if we want to compute the approximate solution over a large interval. This phenomenon led Dahlquist [1] to introduce a special requirement, A-stability;

Definition: A k-step method is called A-stable , if all solutions of the method tend to zero, as $n \to \infty$, when the method is applied with fixed positive h to any differential equation of the form

(1.2) $$d\vec{x}/dt = q\,\vec{x}$$

where $q \in C$ and $\mathrm{Re}\, q < 0$.

In many applications this is a very desirable property, but Dahlquist [1] shows that among all linear multistep methods whith this property, the trapezodial rule is the most accurate.

In order to achieve greater accuracy and order we are then obliged to study non-linear methods, or methods with non-constant coeffisients.

We will now show how the Adams - Bashforth's method

(1.3) $$y_{n+1} = y_n + h \sum_{m=0}^{q} \gamma_m \nabla^m f_n$$

(1.4) $$\gamma_m = (-1)^m \int_0^1 \binom{-s}{m} ds$$

can be made A-stable with a very little modification.

2. Derivation of the formula.

Linear multistep methods may be characterized in that they integrate exactall differential equations of the form

(2.1) $$y^1(x) = T(x)$$

where $T(x)$ is an arbitrary polynomial up to a certain degree. We will instead demand the method to integrate exact the more general class of differential equations

(2.2) $$y^1(x) = -P\, y(x) + T(x)$$

where P is a constant.

The whole idea is now to approximate the function $y^1(x) + P\, y(x)$ with the Lagrangian interpolation polynomial

at the points x_{n-i} , $i = 0, 1, \ldots, q$.

$$(2.3) \qquad T(x) = \sum_{m=0}^{q} (-1)^m \binom{-s}{m} \nabla^m (f_n + Py_n), \quad s = \frac{x-x_n}{h}$$

Next we integrate the equation

$$(2.4) \qquad y'(x) + Py(x) = T(x)$$

with $T(x)$ given by (2.3), between x_n and x_{n+1} to get

$$(2.5) \qquad y_{n+1} = e^{-Ph} y_n + h \sum_{m=0}^{q} s_m \nabla^m (f_n + Py_n)$$

where

$$(2.6) \qquad s_m = (-1)^m e^{-Ph} \int_0^1 e^{Phs} \binom{-s}{m} ds .$$

In order to find a recurrence relation, numerical values and other properties of the coefficients s_m we use the method of generating functions. Let therefore

$$(2.7) \qquad N(t) = \sum_{m=0}^{\infty} s_m t^m .$$

Using (2.6) we find

$$(2.8) \qquad N(t) = e^{-Ph} \cdot \frac{e^{Ph \cdot (1-t)^{-1} - 1}}{Ph - \ln(1-t)}$$

Expanding $(1-t)^{-1}$ and $\ln(1-t)$ in powerseries we obtain

$$(2.9) \qquad s_0 = - \frac{e^{-Ph} - 1}{Ph}$$

$$(2.10) \qquad s_n = - \frac{1}{Ph} \left\{ \sum_{i=1}^{n} \frac{s_{n-i}}{i} - 1 \right\}$$

for the coefficients s_m in (2.6).

From (2.9) and (2.10) we now see that s_m is dependent of h and P . But the calculation of s_n is not hard; we have only to evaluate e^{-Ph} , and then a calculation simular to that for γ_m gives s_m .

So far we have not said anything about the quantity P . The question is ; how to choose P so our new method will be

A-stable. To obtain this, let P be an approximation to $\partial f/\partial y\ (x_n,y_n)$. If we have a single equation

$$y' = f(x,y)\ ,\quad y(a) = \eta$$

a natural choice of P is

$$P = -\frac{f_n - f(x_n,y_{n-1})}{y_n - y_{n-1}} \tag{2.11}$$

However, with this choise of P , we have to evaluate the function f at the point (x_n,y_{n-1}) ; if f is a complicated function, the time used for this extra evaluation may be rather high.

For a system of equations, the choice may depend on the efficiency of the routine to evaluate e^{-Ph} when P is a matrix.

We then have the following theorem,

Theorem: The method (2.5) is A-stable.

Proof: Let $\vec{f}(x,\vec{y}) = q\vec{y}$ with $q \in C$, and $\mathrm{Re}\ q < 0$. Then with $P = -q$, $f_{n-i} + Py_{n-i} = 0$. Q.E.D.

3. The truncation error.

The truncation error, R_q^{SA} of the method is defined to be

$$R_q^{SA} = y(x_{n+1}) - e^{-\tilde{P}h}\, y(x_n) - h\sum_{i=0}^{q} \tilde{s}_m \nabla^m (f(x_n,y(x_n)) + \tilde{P}y(x_n)) \tag{3.1}$$

(See Henrici [2] p.p. 203.) Where, if x is dependent of y_n, $\tilde{x} = x(y(x_n))$.

We will assume that the choice of P is such that

$$\tilde{P} = -f_y(x_n,y(x_n)) + O(h) \tag{3.2}$$

Then we easily find

$$(3.3) \qquad \tilde{s}_m = \gamma_m + O(\tilde{Ph})$$

Using the error term of the Lagrangian interpolation polynomial, (3.2) and (3.3) we find

$$(3.4) \quad R_q^{SA} = h^{q+2}(y^{(q+2)}(x_n) - f_y(x_n, y(x_n))y^{(q+1)}(x_n)) \cdot \gamma_{q+1} + O(h^{q+3}) .$$

4. Concluding remark.

i) The method is A-stable and non-linear.

ii) The order is $q + 1$, as for Adams-Bashforth's method, and the error constant is of the same order as γ_{q+1} which tends to 0 as $q \to \infty$.

iii) When $P = 0$ the method is equal to Adams-Bashforth's method.

This new method with $q = 4$ has been tested at the problem

$$y' = -\left(\frac{1}{(x+1)(x+2)} + 2x\right)y + \frac{x+1}{x^2+1}\left(\frac{1}{(x+1)(x+2)} + 2x\right) + \frac{1-2x-x^2}{(x^2+1)^2}, \quad y(0) = 1$$

because this differential equation gives the same numerical difficulties as stiff equations do. The integration interval was $[0, 100]$. Working with a relative error 10^{-4}, I could start with $h = 0.25$ and increase h to 2 with $P \approx 200$ at $x = 100$. That's $ph \approx 400$, which we could never obtain with Adams-Bashforth's method.

The same problem has as well been integrated by Adams-Bashforth's method, $q = 4$. In this case we had to use $h \approx 10^{-3}$, and if the integrationtime with our new method was t, it now increased to about $3t$ in the smaller intervals $[0,15]$.

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